

Tocopherol-«beta»-tms-derivative (high mass adjustment=0 %)

Other names:	Tocopherol-«beta»-tms-derivative (high mass adjustment=50%) .beta.-Tocopherol, O-trimethylsilyl-
Inchi:	InChI=1S/C31H56O2Si/c1-23(2)14-11-15-24(3)16-12-17-25(4)18-13-20-31(7)21-19-28-2
InchiKey:	LNMHIGHVNIRZML-UHFFFAOYSA-N
Formula:	C31H56O2Si
SMILES:	Cc1cc(O[Si](C)(C)C)c(C)c2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]:	488.86
CAS:	10569-51-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.75		Crippen Method
logp	10.040		Crippen Method
rinpol	2987.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10569514&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/97-205-7/Tocopherol-beta-tms-derivative-high-mass-adjustment-0.pdf>

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